Ising model (cont'd)

PHYS 250 (Autumn 2018) – Lecture 7

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Outline

1. *Reminders*
   - How did we get here and where are we going?
2. *Analytical Ising model*
   - Reminder of statistical mechanics properties
   - 1D Ising Model
   - 2D Ising Model
3. *Ising model observables and calculations*
   - Equilibrium
   - Energy
   - Magnetization
   - Correlations
   - Phase transition
4. *Metropolis Algorithm*

Outline of the Ising model discussion

We've already discussed a lot, and I want to remind you of those topics, their progression, and where we're going from here to make sure that we're all on the same page.

- **Lecture 5: the model iteself**
  - The general concept of the model: lattice of spins
  - Basis in thermodynamics and quantum mechanics
  - Importance of simulations methods
- **Lecture 6: computational approaches**
  - History of computational simulation methods: Monte Carlo
  - The Metropolis Monte Carlo algorithm and its assumptions (deeply related to thermodynamics)
- **Lecture 7 (Today): analytical and computational evaluation**
  - Analytical Ising model and the key numerical results
  - Concept of equilibrium and how we can define it
  - Observables in the Ising model and their calculation
- **"Lecture 8" (Tomorrow): Hands-on lab+lecture**
  - Hands-on session in CSIL 2 for developing our Ising model simulation

Outline

Recall our discussion of statistical mechanics

We discussed that the probability distribution of an observable such as the mean energy, $\langle E \rangle$, of a system in a particular microstate μ is given by

$$\langle E \rangle = \frac{\sum_\mu E_\mu e^{-\beta E_\mu}}{\sum_\mu e^{-\beta E_\mu}} = \frac{\sum_\mu e^{-\beta E_\mu}}{Z} \quad (1)$$

where Z is the **partition function** of the system.

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$$\sum_\mu E_\mu e^{-\beta E_\mu} = -\sum_\mu \frac{\partial}{\partial \beta}\left(e^{-\beta E_\mu}\right) = -\frac{\partial Z}{\partial \beta} \tag{2}$$

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Similarly, the variance is given by:

$$Var(E) = \langle E^2 \rangle - \langle E \rangle^2 = -\frac{\partial \langle E \rangle}{\partial \beta} = \frac{\partial^2 \ln Z}{\partial \beta^2} \quad (4)$$

Ising's analytic solution for a 1D spin lattice (I)

For a single dimension, and just $N = 2$ spins (the smallest possible Ising chain model) we can use the analytic form on the previous slide to write down Z exactly, and thus the mean energy (recall $E = -J \sum_{\langle ij \rangle} s_i s_j$) and its variance.

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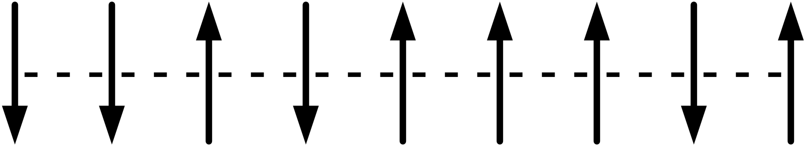

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We can generalize this to N spins, either by induction based on one more manual sum with $N = 3$, or by direct proof (which I leave to you!)

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$$Z_N = \left(2\cosh\beta J\right) Z_{N-1} \tag{14}$$

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Z_N &= (2\cosh\beta J)\, Z_{N-1} && (14)\\
&= (2\cosh\beta J)^N && (15)
\end{aligned}
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(Since $Z_1 = \sum_{s_1=\pm1} 1 = 2$)

Results using Ising's analytic model (I)

With the expression for Z, we can calculate key properties of the system

$$\langle E \rangle = -\frac{1}{Z}\frac{\partial Z}{\partial \beta} = -\frac{\partial \ln Z}{\partial \beta} \tag{16}$$

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$$= -NJ\tanh \beta J \tag{19}$$

Results using Ising's analytic model (II)

Without completing a more thorough derivation, here are three more key properties of the system:

- F: **Helmholtz free energy**, measures the useful work obtainable from a closed thermodynamic system at a constant T and volume. Analogous to Gibbs free energy, which does the same at constant pressure.
- C: **Heat capacity**, measures the system's response to changes in T
- M: **Magnetization**, measures the amount of aligned spins in the system

$$
\begin{aligned}
F &= -\frac{1}{\beta}\ln Z = -\frac{N}{\beta}\ln(2\cosh\beta J) && (20)\\
C &= \frac{\partial\langle E\rangle}{\partial T} = \frac{N(\beta J)^2}{\cosh^2\beta J} && (21)\\
M &= -\frac{\partial F}{\partial H} = \frac{N\sinh\beta H}{\sqrt{\sinh^2\beta H + e^{-4\beta J}}} && (22)
\end{aligned}
$$

Note: at constant T, Helmholtz free energy (F) is minimized at equilibrium.

(lack of) Phase transition for 1D model

The last expression for magnetization M, or magnetization per unit particle, $m = M/N$ shows a very important property

$$M = -\frac{\partial F}{\partial H} = \frac{N \sinh \beta H}{\sqrt{\sinh^2 \beta H + e^{-4\beta J}}} \tag{23}$$

- $M = 0$ for $H = 0$ because $\sinh x \approx x$ for small x
- For $H = 0$, $\sinh \beta H = 0$ and thus $M = 0$
- 1D Ising model becomes a ferromagnet only at $T = 0$ where $e^{-4\beta J} \to 0$, and thus $|M| \to 1$ at $T = 0$.

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There is no state above $T = 0$ for which the mean magnetization is non-zero, while at $T = 0$, we see that $M \to 1$ and the system exhibits a phase transition.

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It has already been pointed out by Ising himself[4] that a linear chain of spins is not ferromagnetic. This can easily be verified by calculating the total magnetization with the help of (5) and (8):

$$M = mN \sinh C/(\sinh^2 C + e^{-4K})^{\frac{1}{2}}, \tag{10a}$$

Kramers & Wannier, 1941

Properties of the 2D Ising model

Outline

Equilibrium

So what do we do with our Monte Carlo program for the Ising model, once we have written it? we probably want to know the answer to some questions like ?What is the magnetization at such-and-such a temperature??, or ?How does the internal energy behave with temperature over such-and- such a range?? To answer these questions we have to do two things. First we have to run our simulation for a suitably long period of time until it has come to equilibrium at the temperature we are interested in. This period is called the equilibration time τ_{eq}. Then we have to measure the quantity we are interested in over another suitably long period of time and average it, to evaluate the estimator of that quantity. What exactly do we mean by ?allowing the system to come to equilibrium?? And how long is a ?suitably long? time for it to happen? How do we go about measuring our quantity of interest, and how long do we have to average over to get a result of a desired degree of accuracy? These are very general questions which we need to consider every time we do a Monte Carlo calculation.

?equilibrium? means that the average probability of finding our system in any particular state ? is proportional to the Boltzmann weight $e^{-\beta E_\mu}$ of that state. If we start our system off in a state such as the $T = 0$ (all spins aligned), and

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